

The Impact of Low Octane Hydrocarbon Blending Streams on the Knock Limit of “E85”

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ABSTRACT

Ethanol is a very attractive fuel from an end-use perspective because it has a high chemical octane number and a high latent heat of vaporization. When an engine is optimized to take advantage of these fuel properties, both efficiency and power can be increased through higher compression ratio, direct fuel injection, higher levels of boost, and a reduced need for enrichment to mitigate knock or protect the engine and aftertreatment system from overheating.

The ASTM D5798 specification for high level ethanol blends, commonly called “E85,” underwent a major revision in 2011. The minimum ethanol content was revised downward from 68 vol% to 51 vol%, which combined with the use of low octane blending streams such as natural gasoline introduces the possibility of a lower octane “E85” fuel. While this fuel is suitable for current “ethanol tolerant” flex fuel vehicles, this study experimentally examines whether engines can still be aggressively optimized for the resultant fuel from the revised ASTM D5798 specification.

The performance of six ethanol fuel blends, ranging from 51-85% ethanol, is compared to a premium-grade certification gasoline (UTG-96) in a single-cylinder direct-injection (DI) engine with a compression ratio of 12.87:1 at knock-prone engine conditions. UTG-96 (RON = 96.1), light straight run gasoline (LSRG, RON = 63.6), and n-heptane (RON = 0) are used as the hydrocarbon blending streams for the ethanol-containing fuels in an effort to establish a broad range of knock resistance for high ethanol fuels.

Results show that nearly all ethanol-containing fuels are more resistant to engine knock than UTG-96 (the only exception being the ethanol blend with 49% n-heptane). This allows ethanol blends made with low octane number hydrocarbons to be operated at significantly more advanced combustion phasing for higher efficiency, as well as at higher engine loads.

While experimental results show that the octane number of the hydrocarbon blend stock does impact engine performance, there remains a significant opportunity for engine optimization when considering even the lowest octane fuels that are in compliance with the current revision of ASTM D5798 compared to premium-grade gasoline.

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INTRODUCTION

The Energy Independence and Security Act of 2007 (EISA) mandates significant increases in the use of renewable fuels in the U.S. [1]. The law established a new renewable fuel standard requiring the nation to use 36 billion gallons of renewable fuel per year by 2022. Given that ethanol is the most widely used renewable fuel in the U.S. and production is expected to continue to grow over the next several years, ethanol is likely to make up a significant portion of the renewable fuel mandate. Over 98% of the fuel ethanol consumed in the U.S. is blended with gasoline to create E10-gasoline with up to 10% ethanol. Additional ethanol is exported or used in intermediate ethanol blends or higher level blends for use in flex-fuel vehicles (FFVs). In 2011,

gasoline consumption in the U.S. was just under 140 billion gallons, 13.7 billion gallons of ethanol were produced domestically, over 1 billion gallons of ethanol were exported, and only 0.033 billion gallons of E85 were consumed (<0.2% of ethanol production) [2].

Consumption of E85 is currently limited by the size of the FFV fleet, the number of E85 fueling stations, and unfavorable pricing of E85 (on a cost per unit energy basis). Consumers with FFVs rarely choose E85 due to higher cost per mile with the current pricing structure. In addition there is a reduced mileage range per tank, so consumers need to fill their gas tanks more frequently. While modern FFVs perform adequately on either gasoline or ethanol, or any blend in between, they are often referred to as “ethanol tolerant”

vehicles because there is limited optimization done to take advantage of ethanol's superior antiknock properties [3].

Each FFV sold in the U.S. must be certified on both E85 and gasoline containing no ethanol (E0) for EPA compliance. Data for the city and highway test for model years 2000 through 2012 were mined from the EPA database retained on www.fueleconomy.gov to develop Figure 1. The plot shows the average E85 fuel economy at 73% of the gasoline fuel economy for both the city and highway tests. While the exact properties of the test fuels for these certification tests is unknown, it is common practice to splash blend 85% denatured fuel-grade ethanol in compliance with ASTM D4806 [4] with 15% certification gasoline to net a resulting E81 blend [3] with 70-72% of the energy per unit volume of the base gasoline. As such, the FFV fleet on the whole displays about a 1-3% efficiency advantage with ethanol fueling.

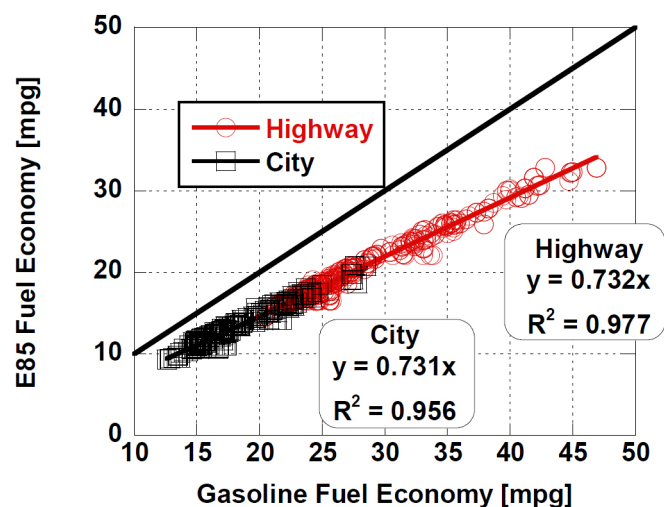


Figure 1. 85 fuel economy versus E0 fuel economy for FFVs (2000-2012) on the city and highway test.

While efficiency increases with E85 are commonly reported, there is not a consensus on the root cause of the efficiency increase. Marriott et al. [5] attributed the efficiency advantage of E85 to a reduction in heat losses due to cooler temperatures, and Szybist et al. [6] found that ethanol led to higher efficiency in a thermodynamic modeling study due to its inherent thermochemical properties. Others attribute the efficiency increase to the way that the engine is operated. For instance, Caton [7] attributed a modest efficiency increase with ethanol to reduced throttling losses on a modeling study of a PFI engine, while on a vehicle level Datta et al. [8] attributed the efficiency increase with E85 primarily to engine calibration differences. Without benchmarking individual vehicles it is not possible to quantify the extent to which the efficiency increases can be attributed to the type of engine calibration differences noted by Dumont et al. [9].

There have been a number of other studies in which engine efficiency has been significantly increased by optimizing the engine hardware to take advantage of the

unique fuel properties of ethanol [10, 11, 12, 13, 14, 15, 16, 17, 18]. While the specifics of the optimization strategies differ somewhat, the premise is to take advantage of the high chemical octane number and high latent heat of vaporization of ethanol by using an engine with high compression ratio, direct injection, and boost. A number of recent studies have highlighted the importance of the latent heat of vaporization of ethanol [14, 15, 16], with Stein et al. [14] finding that the high latent heat of vaporization of ethanol is of equal importance to the overall antiknock behavior as the chemical octane number.

While the optimization potential of high ethanol content fuels is well known, putting an ethanol-optimized vehicle into production necessitates that high quality fuel be widely available. The ASTM D5798 specification for high level ethanol blends, commonly called "E85," underwent a major revision in 2011 [19]. The minimum ethanol content was revised downward from 68 to 51 vol%, and the standard also allows the use of low octane blending streams such as natural gasoline. These changes introduce the possibility of a lower octane "E85" fuel. While this revised fuel is suitable for current "ethanol tolerant" FFVs, this study experimentally examines whether engines can still be aggressively optimized for the resultant fuel from the revised ASTM D5798 specification.

EXPERIMENTAL METHODOLOGY

Single Cylinder Engine

A highly modified 2.0 L GM Ecotec engine with direct fuel injection is used for the study. The engine geometry is listed in Table 1. Three of the cylinders of the production engine are disabled to allow single-cylinder operation. A series of different compression ratio pistons are available for this engine, as was described in an earlier ethanol optimization study with this engine [6], but this study is limited to a single compression ratio of 12.87.

Table 1. Engine geometry

Bore [mm]	86
Stroke [mm]	86
Connecting Rod [mm]	145.5
Compression Ratio [-]	12.87:1
Fuel Injection System	Direct Injection, wall guided

Machining modifications have been made to the cylinder head to accommodate the small research module hydraulic valve actuation (HVA) system from Sturman Industries. Modifications include using custom intake and exhaust valves with extended valve stems. While the valve material is different than the production valves, the combustion chamber geometry is unchanged. Other changes to the engine include a Kistler sparkplug with an integrated piezoelectric pressure transducer. In the production configuration from the original equipment manufacturer (OEM), the high pressure fuel pump for the DI fueling system is driven by the intake camshaft. However, because the camshafts are removed, the fuel is

supplied by an externally powered fuel pump. A picture of the engine research platform used in this investigation is shown in [Figure 2](#).

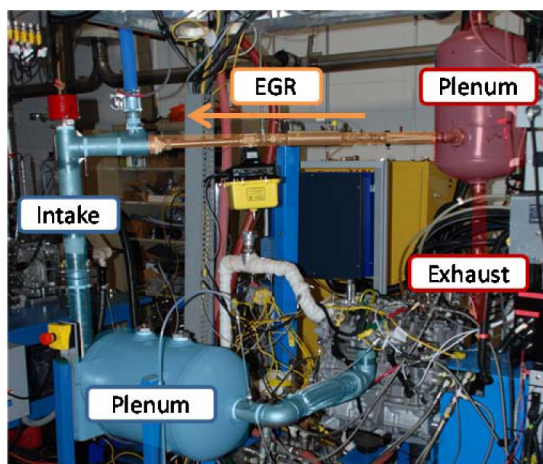


Figure 2. Single cylinder engine equipped with HVA valve train and laboratory air handling system.

The HVA system from Sturman Industries allows independent control of each of the two intake and two exhaust valves, including opening and closing crank angle, opening duration and valve lift, including the option to disable a valve. The intake and exhaust valve timings are held constant at all operating conditions in this study, as shown in [Table 2](#). It should be noted that the valve events produced by this valvetrain are more similar to square waves than a conventional cam-based valve train as was documented in a previous study with this engine [20].

Table 2. Operating conditions.

Valve train	
Intake Valve Opening [CAD] ^{1,2}	-355
Intake Valve Closing [CAD] ^{1,2}	-170
Intake Valve Lift [mm]	9
Exhaust Valve Opening [CAD] ^{1,2}	190
Exhaust Valve Closing [CAD] ^{1,2}	350
Exhaust Valve Lift [mm]	9
Fueling	
Equivalence Ratio	1.0
Fuel injection type	Wall-guided DI
Fuel injection timing [CAD] ¹	-280
Fuel rail pressure [bar]	100
Operating temperatures	
Intake manifold air [deg C]	52
Engine coolant [deg C]	90
Engine oil [deg C]	90

1. 0 CAD represents firing TDC

2. Opening and closing angles at 0.8 mm lift

DRIVEN Combustion Analysis Toolkit (DCAT) performs the crank-angle resolved data acquisition and combustion analysis. These measurements include cylinder

pressure, intake and exhaust valve lift feedback from each of the four valves and the command signal sent to the fuel injector. Crank-angle resolved data is recorded at 0.2 crank angle degree (CAD) intervals.

Engine emissions are measured using a standard emissions bench. NO_x is measured using a chemiluminescence analyzer, CO and CO₂ are measured using infrared analyzers, oxygen is measured using a paramagnetic analyzer and unburned hydrocarbon emissions (HC) are measured with a flame ionization detector. Smoke measurements are performed using a filter smoke number (FSN) instrument. Fuel flow is measured using a coriolis-effect based flow meter.

The engine is operated with a laboratory air handling system. Pressurized air is metered to the engine using a mass air flow controller. Backpressure is applied to the exhaust manifold at the boosted operating conditions using an electromechanically actuated valve so that a constant differential of 10 kPa is maintained between the intake and exhaust manifolds. For example, an intake manifold pressure of 110 kPa has an exhaust manifold pressure of 120 kPa. While this engine platform is equipped with an external exhaust gas recirculation (EGR) system, no EGR is used in this study. The exhaust gas temperature is measured in the exhaust manifold directly after the exhaust port.

Fuel Properties

A total of seven fuel blends are investigated, with full fuel properties listed in [Table 3](#). UTG-96 is a premium-grade certification gasoline procured from CP-Chem. The E85 is a pre-blended product that was also procured from CP-Chem, and as a result, the composition of the hydrocarbon portion of the E85 is unknown. The remaining fuel blends, EB-1 through EB-5, are splash-blended on-site with chemically pure anhydrous 200-proof ethanol and one of three hydrocarbon streams. EB-1 is a blend of UTG-96 with 51 vol % ethanol. EB-2 and EB-3 are ethanol blends with LSRG (antiknock index (AKI) = 63.6) containing 67 and 51 vol% ethanol, respectively. Although it was not investigated in its pure form, the fuel properties of LSRG are included in [Table 3](#). EB-4 and EB-5 are blends of n-heptane (AKI = 0) with 67 and 51 vol% ethanol, respectively. The fuel blends investigated are shown graphically in [Figure 3](#).

LSRG is typically the lowest octane number stream available in high volume at a refinery for gasoline blending [21]. Natural gasoline, the C5-C7 liquid associated with natural gas production, is similar in composition to LSRG and may also be widely available to blend with ethanol given the recent increases in natural gas production in the U.S. It is interesting that the blends made with light LSRG (EB-2 and EB-3) have a resultant research octane number (RON) that is greater than 100. EB-4, which contains 33 vol% n-heptane, also has a RON greater than 100. This result is due to the well-established non-linear response of octane number with ethanol blending on a vol% basis [22, 23], the implications of

Table 3. Fuel properties

	Spec	UTG-96	LSRG	E85	EB-1	EB-2	EB-3	EB-4	EB-5
Hydrocarbon Type	--	UTG-96	LSRG	Unknown	UTG-96	LSRG	LSRG	n-heptane	n-heptane
Ethanol content [vol%]	ASTM D5599	†	†	89.3	52.3	68.9	52.2	67.4	47.3
Reid Vapor Pressure [psi]	ASTM D5191	8.90	12.40	5.12	8.68	8.09	9.34	3.44	3.68
Oxygen content [wt%]	ASTM D5599	†	†	31.22	18.76	25.24	19.65	24.56	17.67
Carbon wt%	ASTM D5291	86.83	84.67	56.22	67.83	60.82	65.62	61.45	66.82
Hydrogen wt%	ASTM D5291	13.20	15.62	12.92	13.10	13.78	14.28	13.92	14.48
Specific Gravity	ASTM D4052	0.739	0.658	0.788	0.768	0.753	0.732	0.756	0.738
Octane nr (R+M)/2	N/A	92.2	63.6	96.9	97.5	96.5	95.0	93.3	81.2
Research Octane Number	ASTM D2699	96.1	64.7	105.0	104.4	104.1	102.0	100.4	84.8
Motor Octane Number	ASTM D2700	88.2	62.4	88.7	90.5	88.9	88.0	86.2	77.6
Octane Sensitivity	N/A	7.9	2.3	16.3	13.9	15.2	14	14.2	7.2
Lower heating value/MJ/kg	ASTM D240	43.286	45.020	29.051	34.186	31.608	34.363	32.103	35.092
Stoichiometric AFR/-	N/A	14.42	14.94	9.45	11.45	10.58	11.57	10.72	11.94
Initial Boiling Point [°C]	ASTM D86	33.9	35.6	†	35	41.1	40.6	70.6	70.6
10% Distillation [°C]	ASTM D86	50.0	47.8	†	57.2	55.0	50.6	71.1	71.1
50% Distillation [°C]	ASTM D86	107.2	57.8	†	76.7	76.7	67.8	73.3	71.1
90% Distillation [°C]	ASTM D86	150.0	76.1	†	89.4	77.8	77.8	77.8	76.1
Final Boiling Point [°C]	ASTM D86	185.0	102.8	†	168.3	78.9	78.9	77.8	78.3
Saturates [vol%]	ASTM D1319	68.0	95.2	†	†	†	†	†	†
Olefins [vol%]	ASTM D1319	2.4	3.3	†	†	†	†	†	†
Aromatics [vol%]	ASTM D1319	29.6	1.4	†	†	†	†	†	†

† Not measured

which are considered further in the Discussion section. EB-5 is the only ethanol-containing blend that resulted in a lower RON than UTG-96 (RON = 84.8). As a result of its low octane number, EB-5 was extremely prone to engine knock and could only be operated at very light engine loads. EB-5 is therefore not included in the results section. It is being included in the fuel properties table because it remains an interesting data point from a blending perspective.

content requirements of ASTM D5798, no attempt was made to comply with the Reid vapor pressure (RVP) requirements. The minimum RVP for compliance with ASTM D5798 is 5.5 psi [19], a requirement that neither EB-4 nor EB-5 are able to meet. In order to comply with the RVP requirements, more volatile hydrocarbons would need to be used which would necessarily increase the AKI of the fuel blend. It is also interesting to note that the pre-blended E-85 is also unable to meet the minimum RVP specification. Volatility is important from a cold-start and driveability perspective, but RVP would not be expected to affect any of the results reported here.

Operating Conditions

This study is focused on the knock-prone portion of the engine operating map, which occurs at low speed and high load. The experimental space includes engine loads of 800, 1000, 1200, and 1400 kPa IMEP_{net} at engine speeds of 1500, 2000, and 2500 rpm. The maximum load is limited to 1400 kPa IMEP_{net} because higher engine loads approach the 100 bar cylinder pressure limitation for this engine with the high compression ratio configuration used in this study. 1200 kPa IMEP_{net} is nominally the engine load achieved at wide open throttle conditions, although it is dependent of fuel. For fuels capable of achieving 1200 kPa IMEP_{net} with an intake manifold pressure of less than 98 kPa, there is no added backpressure. If the intake manifold pressure is 99 kPa absolute or higher, the exhaust manifold pressure is maintained at a pressure of 10 kPa higher than the intake manifold to simulate a turbocharger. It is necessary to boost

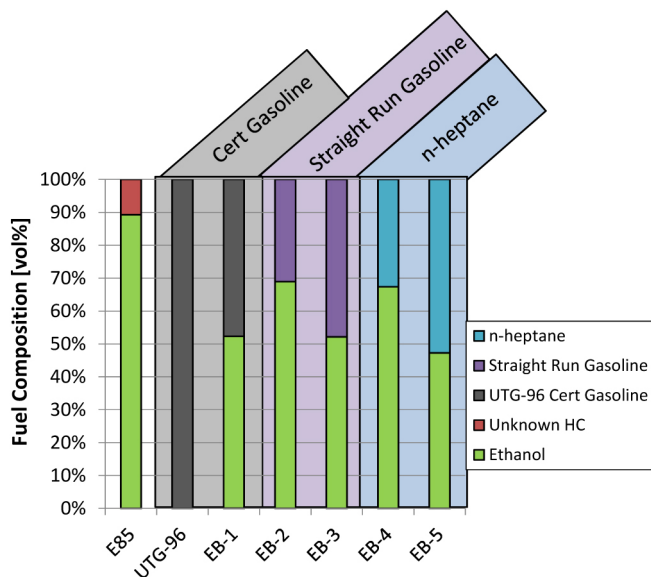


Figure 3. Composition of fuel blends investigated.

It is also interesting to note that while the fuel blends selected in this study are intended to comply with the ethanol

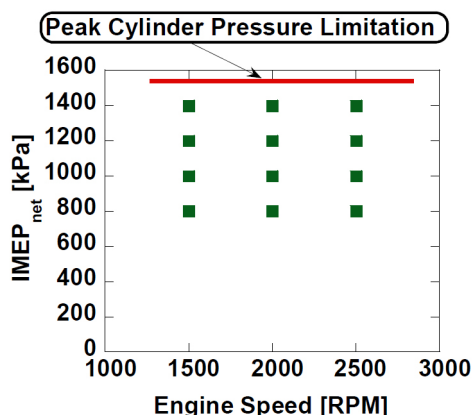


Figure 4. Engine operating points investigated.

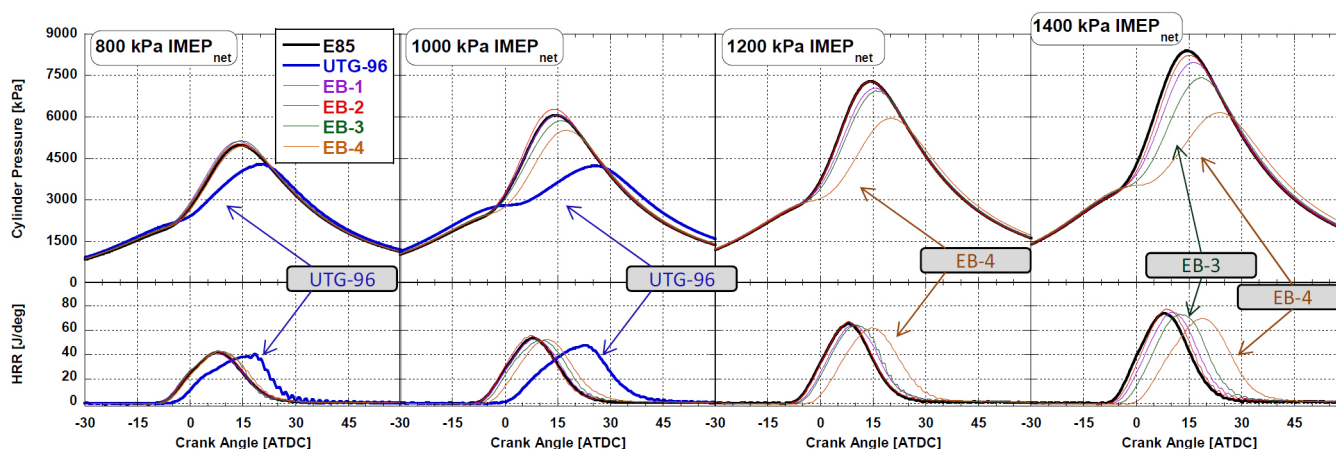


Figure 5. Cylinder pressure and heat release rate at 2000 rpm.

intake pressure to reach 1400 kPa $IMEP_{net}$ for all fuels. The operating conditions are shown graphically in Figure 4.

Spark timing is adjusted to keep the combustion midpoint timing (CA_{50}) relatively constant, at a timing of 8-9 CAD after firing top dead center ($aTDC_f$) except at conditions where it is necessary to retard combustion phasing to mitigate knock. Combustion phasing of 8-9 CAD $aTDC_f$ corresponds to the optimal maximum brake torque (MBT) combustion phasing. For the purposes of bounding this study and preventing damage to the engine, exhaust gas temperature is limited to 725°C and CA_{50} combustion phasing is limited to 25 CAD $aTDC_f$.

RESULTS

Combustion Phasing

Cylinder pressure and heat release rate are shown in Figure 5 for each engine load at 2000 rpm. At the lightest load investigated, 800 kPa $IMEP_{net}$, there is very little difference between the ethanol-containing fuels because they can all be operated at the targeted combustion phasing without knock ($CA_{50} = 8-9$ CAD $aTDC_f$). However, the

phasing of UTG-96 is knock-limited, so it is significantly more retarded than the ethanol-containing fuels.

As engine load is increased to 1000 kPa $IMEP_{net}$, the knock limitations for UTG-96 are more pronounced, requiring its combustion phasing to be retarded further than at the 800 kPa $IMEP_{net}$ condition. Engine load cannot be increased higher than 1000 kPa $IMEP_{net}$ for UTG-96 because of the CA_{50} combustion phasing limit of 25 deg $aTDC_f$. As a result, the knocking tendency of UTG-96 limits its peak load while ethanol-containing fuels can utilize the boosted air handling system of the engine to achieve higher engine load and torque, as is required by modern downsized and down-speeded engines.

While E85 and EB-1 through EB-4 are all more resistant to knock than UTG-96, Figure 5 does show that knock-resistance differences do exist for the ethanol-containing fuels. At an engine load of 1000 kPa $IMEP_{net}$ and higher, the combustion phasing for EB-4 is retarded because of knock limitations, and phasing for EB-3 is knock-limited at an engine load of 1400 kPa $IMEP_{net}$.

While the cylinder pressure and heat release in Figure 5 are informative, Figure 6 presents a more complete

assessment of knock-limited combustion phasing across the range of speed and load investigated. CA50 combustion phasing is shown as a function of engine load at the three different engine speeds. The target combustion phasing of 8-9 CAD aTDC_f is highlighted in gray for each engine speed, and the operating points outside of the gray box are knock-limited. Knocking tendency becomes more severe as engine load increases and as engine speed decreases, consistent with the established behavior of engine knock.

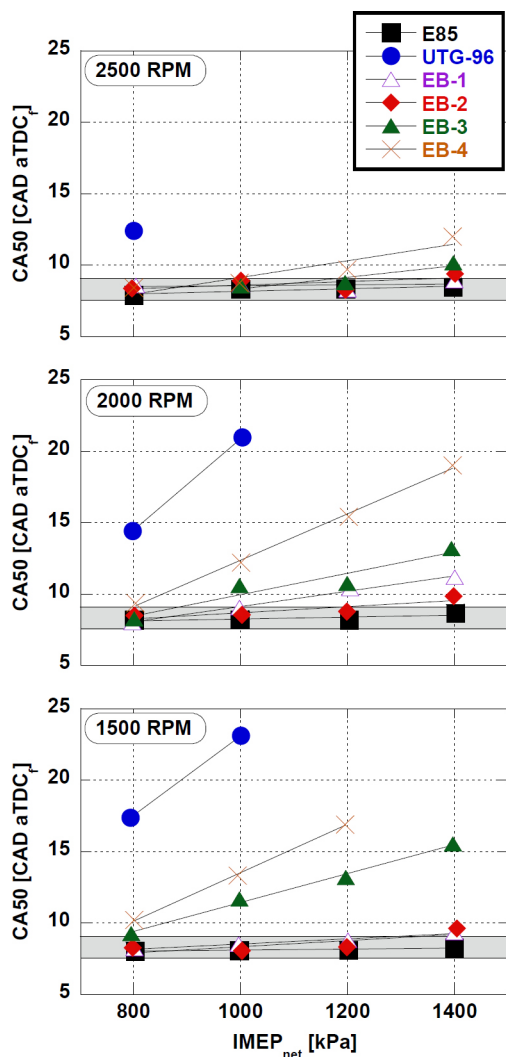


Figure 6. Combustion phasing as a function of engine load.

As was also observed in Figure 5, UTG-96 is the most severely knock-limited fuel regardless of engine speed. Engine load is limited to 1000 kPa IMEP_{net} at 1500 and 2000 rpm for UTG-96 because of the combustion phasing limitation, and is limited to 800 kPa IMEP_{net} at 2500 rpm because of the exhaust temperature limitation of 725°C. As a result, the knocking behavior of UTG-96 is a significant limitation to its peak load compared to the ethanol-containing fuels.

Combustion phasing for EB-3 and EB-4 is significantly knock-limited at the highest load conditions at 1500 and 2000 rpm. Thus, while these fuels offer improved performance compared to UTG-96, a premium grade certification gasoline, the hydrocarbon type and the ethanol content does influence the knock-resistance of the high ethanol content fuel blends.

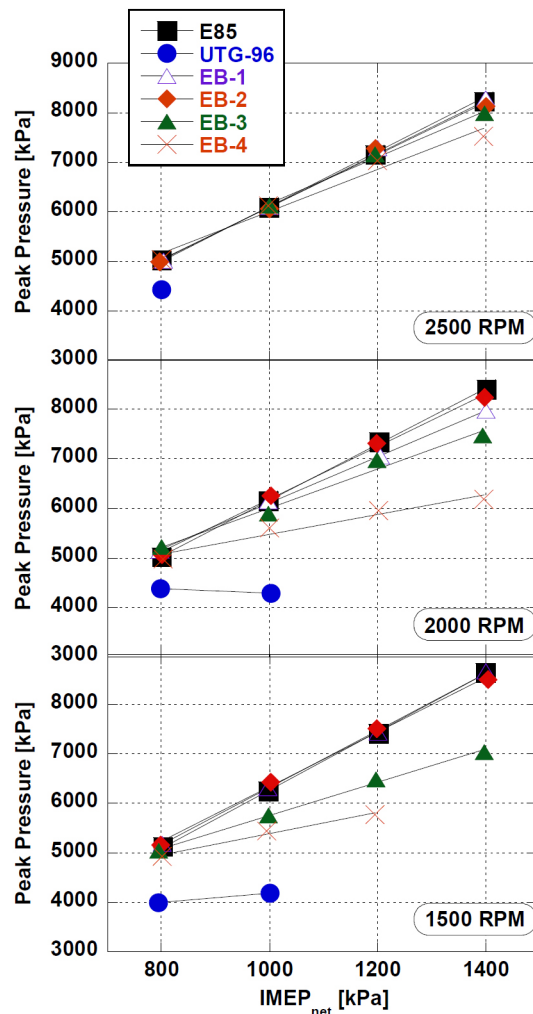


Figure 7. Peak cylinder pressure as a function of load.

Retarding combustion phasing is an effective means of mitigating engine knock, but it is thermodynamically undesirable because of its effect on the peak cylinder pressure and thermal efficiency. Figure 7 shows the relationship between peak cylinder pressure and engine load. For the fuels that are not knock-limited, peak cylinder pressure naturally increases with engine load due to a combination of higher intake manifold pressure and an increase in fuel energy released. However, for fuels with knock-limited combustion phasing, the peak cylinder pressure is significantly reduced. This observation is particularly notable for UTG-96 which has the most retarded combustion phasing. For example, the peak cylinder pressure for UTG-96 (approximately 4000 kPa)

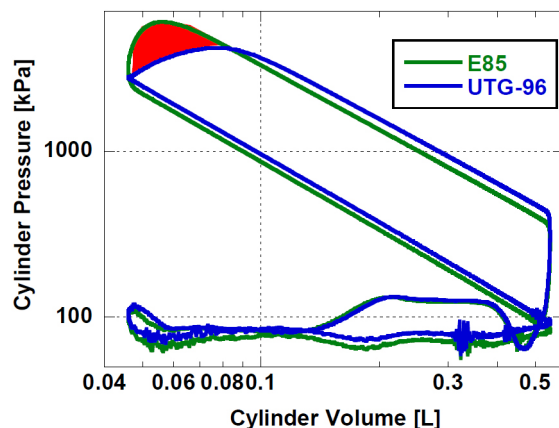


Figure 8. P-V Diagram of E85 and UTG-96 at 2000 rpm, 10 bar $IMEP_{net}$

is nearly one-third lower than for E85 (approximately 6000 kPa) at 1500 rpm, 1000 kPa $IMEP_{net}$.

The thermodynamic penalty associated with the retarded combustion phasing and reduced peak cylinder pressure is illustrated in a PV diagram for E85 and UTG-96 in Figure 8. The more advanced combustion phasing and higher peak pressure for E85 allow the expansion stroke to be nearly fully utilized to produce piston work. In contrast, because of the retarded combustion phasing and reduced peak cylinder pressure, a significant portion of the expansion stroke is underutilized for UTG-96, as is indicated by the portion of the diagram highlighted in red. As a result of this underutilization, more fuel and air is required to maintain the same load. Evidence of the need for more fuel and air is the higher pressure for UTG-96 during the intake stroke, compression stroke, and late in the expansion stroke.

Fuel Consumption and Efficiency

Net indicated thermal efficiency (ITE_{net}) as a function of engine load is shown in Figure 9. The general behavior at all engine speeds is for ITE_{net} to increase with engine load from 800 to 1200 kPa $IMEP_{net}$ due to a reduction in throttling losses and lower heat losses per unit mass, then it is approximately constant at 1200 and 1400 kPa $IMEP_{net}$ where pumping work remains approximately constant.

For the fuels that do not have knock-limited combustion phasing at any of the operating conditions (E85, EB-1, and EB-2) there are few differences in ITE_{net} , with these fuels being within one efficiency point of each other. In contrast, there is a reduction in ITE_{net} for fuels with knock-limited combustion phasing. This characteristic can be observed at 1500 rpm 1200 kPa $IMEP_{net}$ for EB-4, and at 2000 rpm at 1400 kPa $IMEP_{net}$ for both EB-3 and EB-4. It is most notable for UTG-96, however, where ITE_{net} is between 2 and 3 efficiency points lower than the ethanol blends due to its severely retarded combustion phasing.

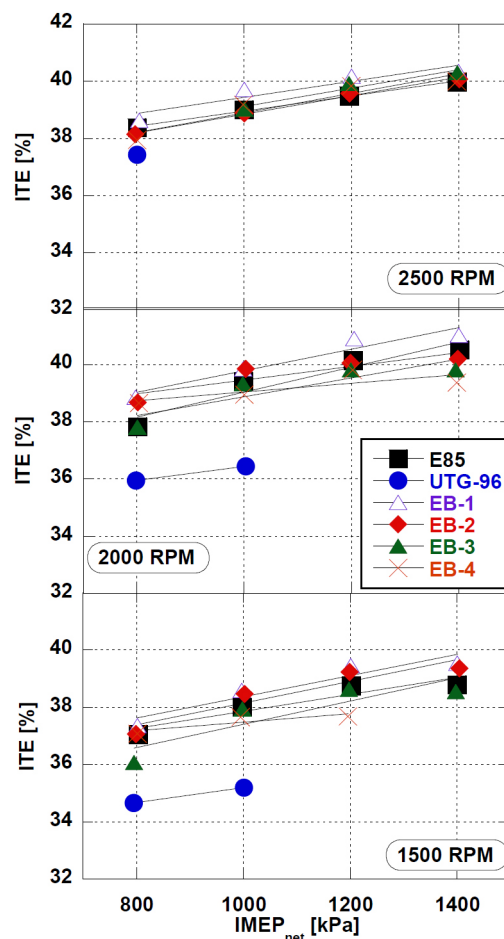


Figure 9. Net indicated thermal efficiency as a function of engine load.

Despite its lower thermal efficiency, UTG-96 has the lowest specific fuel consumption on a mass basis as shown in Figure 10. This result is because specific fuel consumption is dominated by the lower heating value of the fuel, with clear groupings observed with the ethanol content of the fuels. The differences in LHV are significant, with E85 having an LHV

that is nearly 33% lower than UTG-96, so while the ITE_{net} benefit of 2-3 efficiency points is significant, it is masked by the larger differences in heating value. As ethanol content is reduced to 67% (EB-2 and EB-4) and 51% (EB-1 and EB-3), there is a smaller LHV penalty compared to E85, and as a result a reduced specific fuel consumption penalty.

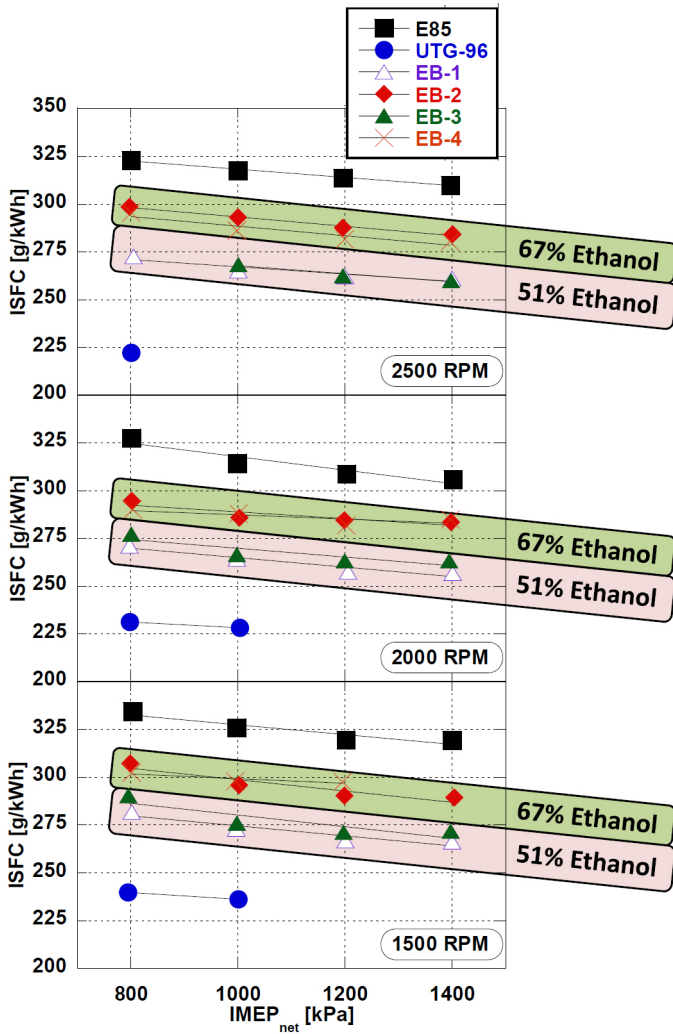


Figure 10. Indicated specific fuel consumption as a function of engine load.

DISCUSSION

Octane Number

The results in this study illustrate the potency of ethanol as an octane number improver. Of particular note is that EB-2 through EB-4 contain high concentrations of LSRG (RON = 64.7) and n-heptane (RON = 0), but result in fuel blends with RON > 100 as is shown in Table 3.

It is well-established that the octane number response with volumetric ethanol blending is non-linear [10, 14], with nearly two-thirds of the octane number improvement being realized for a one-third ethanol volumetric blend. Anderson et

al. [22, 23] investigated the root-cause of this behavior and concluded that the octane number response is approximately linear on a mole fraction basis with ethanol. Because ethanol has a molecular weight that is less than half the average molecular weight of gasoline, the mole fraction of ethanol is much higher than the volumetric blending fraction.

One implication of this finding is that there is a potential to use ethanol to upgrade low-cost refinery blending streams. This approach appears to be common practice with the production of blendstock for oxygenate blending (BOB) for E10. The E10 currently sold throughout most of the U.S. meets the required octane number only after getting the octane number benefits of the 10 vol% ethanol, whereas gasoline not containing any ethanol has to meet the octane number requirement and did so routinely for years before blending with 10 vol% ethanol was nearly ubiquitous. Utilizing the octane number boost with E10 is a logical approach for refiners because producing hydrocarbon streams with high octane number fuel is expensive, and there is no motivation to “give away” octane.

An alternate implication of the non-linear octane number response with vol% ethanol is that there is the potential to optimize an engine for ethanol blends that contain significantly less than 85% ethanol. From a realistic standpoint, EB-3 (RON = 102) is representative of the lowest octane number fuel blend that could enter the marketplace and still comply with the ethanol content and RVP requirements of ASTM D5798. The octane number of high ethanol blends can be reduced to much lower levels, as illustrated by EB-5 (RON = 84.4), but this requires relatively heavy hydrocarbons, and the resultant fuel blend will not meet the minimum RVP specification of 5.5 psi (EB-5 RVP = 3.68 psi). Blending with lighter hydrocarbons to comply with the RVP specifications will have the additional result of increasing the octane number because octane number increases as molecular weight decreases for a given class of hydrocarbon. As a result, refiners necessarily “give away” octane for fuels compliant with ASTM D5798. In addition, it is likely that fuel blends containing 30-50 vol% ethanol could have significant optimization potential when blended with hydrocarbon blendstocks with modest octane number (RON 75-80).

Vehicle Optimization

This study illustrates many of the thermodynamic efficiency benefits that can be realized with an ethanol-optimized engine configuration. However, there are additional system-level benefits that can be exploited for further real-world miles-per-gallon gains on a fully ethanol-optimized vehicle. The two aspects that will be discussed here are that ethanol can be an enabler to down-speeding and downsizing, and the lower exhaust temperature for ethanol can reduce the fuel consumption because of a reduced need for fuel enrichment.

Down-speeding and downsizing

At the high compression ratio engine configuration used in this study, the knocking behavior of UTG-96 limits the maximum load to 1000 kPa IMEP_{net} at 1500 and 2000 rpm, and 800 kPa IMEP_{net} at 2500 rpm. In contrast, all of the ethanol fuel blends could achieve an engine load of 1400 kPa IMEP_{net}, and likely could have operated at higher engine load if it had not been limited by the peak cylinder pressure of the engine.

Thus, ethanol fuels have the ability to deliver a higher load at the low engine speeds, or have improved low-end torque. When matched with the appropriate transmission gear ratio, the engine can be operated at lower speed and higher torque than with gasoline for a given demanded power, ultimately allowing the engine to produce power at a more efficient operation point. Moore et al. estimated that by down-speeding with a 6-speed transmission, an ethanol-optimized FFV could achieve nearly the same miles-per-gallon as gasoline during the FTP driving cycle [11].

Additionally, because of the higher load capabilities of ethanol fuels, OEMs can be more aggressive with engine downsizing. Downsizing, or replacing a large displacement engine with smaller engine that has a higher specific power output is a leading industry trend to improve fuel economy [24, 25]. The fuel economy benefits of using a downsized engine are well established and are a result of operating engines at higher load to reduce the throttling losses and decrease the engine friction compared to larger displacement engines while using boosted air handling systems to increase the specific power output of the engine. However, it is often necessary to have a reduced compression ratio in downsized applications to mitigate engine knock [26]. Due to both the high chemical octane number and the high latent heat of vaporization of high ethanol-content fuels, high compression ratio can be maintained even under boosted conditions provided that the peak cylinder pressure limit capability of the engine is sufficiently high.

Reduced exhaust temperature

Vehicles with spark ignition engines in the U.S. generally operate with a stoichiometric air-fuel mixture to enable proper operation by the 3-way exhaust catalyst for emission reduction. However, the EPA allows engine manufacturers to use up to 6% enrichment (extra fuel) when necessary in order to cool the exhaust temperature in order to protect the engine or emissions control equipment from overheating [27].

There is a large efficiency penalty for enrichment because very little additional piston work is produced by the excess fuel. The frequency at which vehicles encounter fuel enrichment conditions is not well known across the fleet, and is thought to be highly dependent on the power-to-weight ratio of the vehicle as well as the specific behavior of the driver. However, as the trend of engine downsizing becomes more widespread the dependency on high engine load operating conditions increases.

High ethanol-content fuels can significantly reduce the need for fuel enrichment because they produce a lower exhaust temperature, and as a result enrichment would be required less frequently. Part of the lower exhaust temperature can be attributed to the specific thermochemical properties of ethanol. Ethanol has a high latent heat of vaporization and cools the fuel-air mixture, so the temperature at the start of compression is lowest for high ethanol-content fuels [5]. Additionally, when ethanol is burned, the number of moles created during combustion is substantially higher than for hydrocarbon fuels, and as a result the temperature of the resultant mixture is lower [6].

However, the most significant factor leading to lower exhaust temperatures for high ethanol-content fuels is the combustion phasing difference because of the strong anti-knock characteristics of ethanol. As combustion phasing is retarded to mitigate knock for lower octane gasoline fuels, the exhaust temperature increases while the efficiency decreases. Experimental results from this study, Figure 11, show that the exhaust temperature of gasoline can be more than 60°C higher than for E85, consistent with values previously reported in the literature [5, 10]. Thus, at a high load condition, gasoline can incur one efficiency penalty for retarding the combustion phasing and another efficiency penalty for fuel enrichment, while a high ethanol fuel would not incur any efficiency penalty.

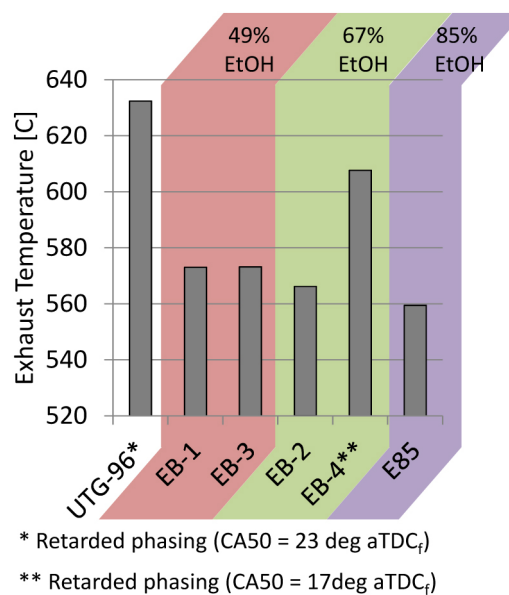


Figure 11. Exhaust temperature at 1500 rpm, 1000 kPa IMEP_{net}

CONCLUSIONS

The primary conclusion of this work is that compared to a premium-grade gasoline, there is a substantial opportunity to optimize engine hardware to improve engine efficiency and performance for any fuel compliant with the "E85" specification, ASTM D5798. The basis of the optimization

potential is the knock resistance of ethanol due to its high chemical octane number and high latent heat of vaporization. Engine hardware modifications include high compression ratio, direct fuel injection, and boosting.

The superior knock resistance of high ethanol-content fuels enables optimal combustion phasing at high load for high compression ratio configurations. In contrast, it is necessary to significantly retard the combustion phasing of premium-grade gasoline in order to mitigate engine knock at this high compression ratio. Retarded combustion phasing incurs an efficiency penalty because it significantly reduces the peak cylinder pressure leading to an underutilization of the expansion stroke. This work illustrated that the peak cylinder pressure was nearly one-third lower for premium-grade gasoline than for the high ethanol-content fuels at some conditions.

The optimization potential of ASTM D5798-compliant fuels is present despite the permitted use of low octane number hydrocarbon blending streams or the allowable use of ethanol concentrations as low as 51 vol%. This observation illustrates the potency of ethanol to boost the octane number. The octane number response with ethanol blending is highly non-linear, with nearly two-thirds of the octane number benefit of ethanol blending realized at a one-third concentration on a volumetric basis. Previous reports in the literature show that the octane number response is nearly linear with the mole fraction of ethanol [22, 23].

The potential thermodynamic benefits of high ethanol-content are substantial, 2-3 efficiency points higher than premium-grade gasoline. On a specific fuel consumption basis, however, the efficiency differences are masked by the larger differences in energy content between the ethanol and the hydrocarbon fuels. Nevertheless, the potential fuel consumption benefits of high ethanol fuel blends extend beyond thermodynamic efficiency alone because there are opportunities to optimize the vehicle system for the ethanol-optimized engine. Particularly, the higher specific power output with high ethanol fuel blends allows engine manufacturers to be more aggressive with downsizing and down-speeding technologies while maintaining a high compression ratio. Additionally, the cooler exhaust temperatures with ethanol, due to more advanced combustion phasing and other fuel-specific properties, can lead to an additional efficiency advantage by reducing the need for fuel enrichment to cool the engine exhaust under high load conditions.

REFERENCES

1. One Hundred Tenth Congress of the United States of America, Energy Independence and Security Act of 2007. 2007; H.R. 6.
2. U.S. Energy Information Administration, *Monthly Energy Review*, DOE/EIA-0035(2012/08), August 2012, available at <http://www.eia.gov/totalenergy/data/monthly/pdf/mer.pdf>
3. West, B., López, A., Theiss, T., Graves, R. et al., "Fuel Economy and Emissions of the Ethanol-Optimized Saab 9-5 Biopower." SAE Technical Paper 2007-01-3994, 2007, doi:10.4271/2007-01-3994.
4. ASTM Standard D 4806-06c, Specification for Denatured Fuel Ethanol for Blending with Gasolines for Use as Automotive Spark Ignition Engine Fuel, Annual Book of ASTM Standards, Vol 05.03.
5. Marriott, C., Wiles, M., Gwidt, J., and Parrish, S., "Development of a Naturally Aspirated Spark Ignition Direct-Injection Flex-Fuel Engine," *SAE Int. J. Engines* 1(1):267-295, 2009, doi:10.4271/2008-01-0319.
6. Szybist, James P., Chakravarthy Kalyana, and Daw C. Stuart, "Analysis of the Impact of Selected Fuel Thermochemical Properties on Internal Combustion Engine Efficiency," *Energy Fuels*, 2012, 26 (5), pp 2798-2810 DOI: 10.1021/1021.
7. Caton, J., "A Thermodynamic Evaluation of the Use of Alcohol Fuels in a Spark-Ignition Engine," *SAE Int. J. Fuels Lubr.* 2(2):1-19, 2010, doi: 10.4271/2009-01-2621.
8. Datta, R., Maher, M.A., Jones, C., and Brinker, R.W., "Ethanol-The Primary Renewable Liquid Fuel," *J. Chem. Technol. Biotechnol.* 86(4): 473-480, 2011, doi: 10.1002/jctb.2580.
9. DuMont, R., Cunningham, L., Oliver, M., Studzinski, M. et al., "Controlling Induction System Deposits in Flexible Fuel Vehicles Operating on E85," SAE Technical Paper 2007-01-4071, 2007, doi: 10.4271/2007-01-4071.
10. Szybist, J., Foster, M., Moore, W., Confer, K. et al., "Investigation of Knock Limited Compression Ratio of Ethanol Gasoline Blends," SAE Technical Paper 2010-01-0619, 2010, doi:10.4271/2010-01-0619.
11. Moore, W., Foster, M., and Hoyer, K., "Engine Efficiency Improvements Enabled by Ethanol Fuel Blends in a GDI VVA Flex Fuel Engine," SAE Technical Paper 2011-01-0900, 2011, doi: 10.4271/2011-01-0900.
12. Christie, M., Fortino, N., and Yilmaz, H., "Parameter Optimization of a Turbo Charged Direct Injection Flex Fuel SI Engine," *SAE Int. J. Engines* 2(1):123-133, 2009, doi:10.4271/2009-01-0238.
13. Milpied, J., Jeuland, N., Plassat, G., Guichaous, S. et al., "Impact of Fuel Properties on the Performances and Knock Behaviour of a Downsized Turbocharged DI SI Engine - Focus on Octane Numbers and Latent Heat of Vaporization," *SAE Int. J. Fuels Lubr.* 2(1):118-126, 2009, doi:10.4271/2009-01-0324.
14. Stein, R., Polovina, D., Roth, K., Foster, M. et al., "Effect of Heat of Vaporization, Chemical Octane, and Sensitivity on Knock Limit for Ethanol - Gasoline Blends," *SAE Int. J. Fuels Lubr.* 5(2):823-843, 2012, doi:10.4271/2012-01-1277.
15. Kasseris, E. and Heywood, J., "Charge Cooling Effects on Knock Limits in SI DI Engines Using Gasoline/Ethanol Blends: Part 1-Quantifying Charge Cooling," SAE Technical Paper 2012-01-1275, 2012, doi: 10.4271/2012-01-1275.
16. Kasseris, E. and Heywood, J., "Charge Cooling Effects on Knock Limits in SI DI Engines Using Gasoline/Ethanol Blends: Part 2-Effective Octane Numbers," *SAE Int. J. Fuels Lubr.* 5(2):844-854, 2012, doi: 10.4271/2012-01-1284.
17. Hoyer, K., Moore, W., and Confer, K., "A Simulation Method to Guide DISI Engine Redesign for Increased Efficiency using Alcohol Fuel Blends," *SAE Int. J. Engines* 3(1):889-902, 2010, doi: 10.4271/2010-01-1203.
18. Stein, R., House, C., and Leone, T., "Optimal Use of E85 in a Turbocharged Direct Injection Engine," *SAE Int. J. Fuels Lubr.* 2(1): 670-682, 2009, doi:10.4271/2009-01-1490.
19. ASTM Standard D5798-11, Standard Specification for Ethanol Fuel Blends for Flexible-Fuel Automotive Spark-Ignition Engines.
20. Weall, A., Szybist, J., Edwards, K., Foster, M. et al., "HCCI Load Expansion Opportunities Using a Fully Variable HVA Research Engine to Guide Development of a Production Intent Cam-Based VVA Engine: The Low Load Limit," *SAE Int. J. Engines* 5(3):1149-1162, 2012, doi: 10.4271/2012-01-1134.
21. Gary, J.H., and Handwerk, G.E. *Petroleum Refining Technology and Economics Fourth Edition*. New York: Marcel Dekker, 2001.
22. Anderson, J.E., Kramer, U., Mueller, S.A., Wallington, T.J., "Octane Numbers of Ethanol - and Methanol - Gasoline Blends Estimated from Molar Concentrations," *Energy & Fuels* 24(12):6576-6585, 2010, doi: 4134154/ef101125c.
23. Anderson, J., Leone, T., Shelby, M., Wallington, T. et al., "Octane Numbers of Ethanol-Gasoline Blends: Measurements and Novel Estimation Method from Molar Composition," SAE Technical Paper 2012-01-1274, 2012, doi:10.4271/2012-01-1274.
24. Han, D., Han, S., Han, B., and Kim, W., "Development of 2.0L Turbocharged DISI Engine for Downsizing Application," SAE Technical Paper 2007-01-0259, 2007, doi:10.4271/2007-01-0259.
25. Lumsden, G., OudeNijeweme, D., Fraser, N., and Blaxill, H., "Development of a Turbocharged Direct Injection Downsizing Demonstrator Engine," *SAE Int. J. Engines* 2(1):1420-1432, 2009, doi: 10.4271/2009-01-1503.
26. Fraser, N., Blaxill, H., Lumsden, G., and Bassett, M., "Challenges for Increased Efficiency through Gasoline Engine Downsizing," *SAE Int. J. Engines* 2(1):991-1008, 2009, doi:10.4271/2009-01-1053.
27. Knoll, Keith, West Brian, Clark Wendy, Graves Ronald, Orban John, Przesmitzki Steve, and Theiss Timothy, *Effects of Intermediate Ethanol Blends on Legacy Vehicles and Small Non-Road Engines*, Report 1-Updated, NREL/TP-540-43543/ORNL/TM-2008/117, February 2009, available at <http://www.nrel.gov/docs/fy09osti/43543.pdf>.

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DEFINITIONS/ABBREVIATIONS

AKI - Antiknock index

BOB - Blendstock for oxygenate blending

CAD - Crank angle degrees

CA50 - Crank angle (timing) of the 50% mass fraction burned

DCAT - DRIVVEN combustion analysis toolkit

EISA - Energy Independence and Security Act of 2007

EPA - U.S. Environmental Protection Agency

FFV - Flex fuel vehicle

FSN - Filter smoke number

FTP - Federal test protocol

HVA - Hydraulic valve actuation

IMEP_{net} - Net indicated mean effective pressure

ITE_{net} - Net indicated thermal efficiency

LHV - Lower heating value

MON - Motor octane number

NO_x - Oxides of nitrogen

OEM - Original equipment manufacturer

RON - Research octane number

RVP - Reid vapor pressure

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